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Quarterly Technical Report

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1. PROGRESS DURING THE REPORTING PERIOD.

1.1 Naval Research Laboratory (NRL):

The CM5, with 128 nodes, was installed at NRL in November of 1992. In late December, the upgrade to 256 nodes and 48 drives of Scalable Disk Array (1 Gigabyte each) was begun. NRL is awaiting native HIPPI. In the late winter the first few users started using the machine. Now there are over 100 users with accounts on the CM5. We discuss some of the projects and their results below.

Inertial Confinement / Laser Fusion:

Jill P. Dahlburg, John H. Gardner, David E. Fyfe (NRL)
and external collaborators

This group has been working on a simulating the full nonlinear evolution of a 3 dimensional Rayleigh-Taylor instability. Their goal is "to obtain predictive capability of how the presence of many RT-unstable modes affect RT single-mode saturation and shape effects, including finite-thickness target information like the target mass ratio $\rho R_{min} / \rho R_{max}$ (what experimentalists can measure) and local minimum values of the mass integral, ρR (of primary interest for target design)". The fast processing and large memory of the CM-5 have allowed them to implement the table look-ups inherent in the real equation of state and the variable Eddington multigroup radiation transport calculations. The efficiency of CM_FORTTRAN library routines minimizes memory usage as well as promoting parallel efficiency. The work has been presented at the 23rd Anomalous Absorption Conference and submitted to the 1993 American Physical Society/Division of Plasma Physics Meeting.

Relevant publications include:

J.P.Dahlburg, J.H.Gardner, S.W.Haan, & G.D.Doolen, Phys.Fluids B, vol 5, 571 (1993).
J.P.Dahlburg, J.H.Gardner, D.E.Fyfe, S.W.Haan, & G.D.Doolen, (in prep., 1993).
J.P.Dahlburg, & J.H.Gardner, Bull.Am.Phys.Soc. vol 37, 1471, (1992).

Weather Prediction:

Paul Anderson, Michael Young, Joseph Bradley, David Norton,
Peter Caress (NRL), Joseph Sela (National Meteorological
Center, National Weather Service)

This group has been converting the NOAA National Weather Service global weather forecast model from a Cray Y-MP/8 version to a Connection Machine version. The code does not yet run on the CM-5 (because of a dependence on the CMSSL FFT routine) but it is expected that performance on the CM-5 will ultimately be good.

A similar conversion of the Navy global spectral weather model is also underway. Activity to date has centered on conversion of the Navy atmospheric physics modules.

Details on their approach to spectral to grid conversion have been

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documented in a paper submitted for a special issue of the Journal of Parallel and Distributed Computing.

High t_c Superconducting:

J.W. Serene and D.W. Hess (NRL)

Using both the CM-200 and CM-5, they are studying Anderson lattice models and Hubbard models, which are believed to contain the essential physics for understanding the role of the strong interactions between electrons in certain rare earth and actinide compounds called heavy electron systems, and in the high temperature superconductors and related transition metal compounds. They have developed a massively parallel code that allows them to solve efficiently the set of nonlinear coupled equations for the self energy in what is known as the fluctuation exchange approximation.

Space Surveillance:

Liam Healy (NRL)

This project is concerned with tracking, cataloging and analyzing the orbital motion of more than 7000 earth-orbiting objects. Orbit propagation, that is, finding a satellite's future position and velocity from its current position and velocity, is an essential component of all aspects of the computing. Parallelizing with one satellite per virtual processor, there is no communication needed, because all satellites evolve independently of one another. Close conjunction determination, finding pairs of satellites that come within a certain distance of another at some point during the orbit, does involve communication but is much faster than on a serial computer. These are now running on the CM-5 and provide capability for studies impossible before. He is now working towards implementation of other space surveillance tasks such as orbit determination, track correlation and object identification.

Finite-Volume Magnetohydrodynamics Codes:

Rick Devore (NRL)

Researchers are implementing a pair of 2.5-dimensional (2-dimensional spatial variations, 3-dimensional vector fields) MHD models using flux-corrected transport (FCT) finite-volume techniques on the CM-5. Efforts to date have focused on developing and optimizing the core FCT modules used to time-advance the generalized continuity and hydromagnetic equations of the models. The modules are written in CM Fortran and have been tested on a simple 2-dimensional blast wave problem using computational meshes of various sizes. TMC's Prism development tool has been used to debug and gather performance statistics from these tests, on both the CM-5 and the CM-200.

Preliminary experiments with the CM-5 suggest that we can expect about 700 MFlops sustained speed on a 256x256 grid, compared with the 150 MFlops obtained on a single-processor Cray Y-MP. This reduces the computation time for a typical simulation from 24 hours to about 5 hours. On a 1024x1024 grid, the communications penalty is smaller and about 3 GFlops can be attained. This much better resolved calculation

would require about 3 days on the CM-5, compared with some 2 months on the Y-MP. The newly released run time system for CM Fortran should substantially improve the performance on the 256x256 problem, whose compute time is overwhelmingly dominated by the required communications (circular shifts). It is hoped that future releases of the Fortran compiler also will be able to take better advantage of the massive parallelism inherent in these codes and achieve more efficient use (than the present 20%) of the fast vector units.

High Speed Combustion Flows:

Elaine S. Oran (NRL), Robert Whaley (TMC) and external collaborators

A computational fluid dynamics (CFD) code capable of simulating unsteady, compressible reactive flows has been developed on the massively parallel Connection Machine. The parallel CFD code, which was written in CM Fortran, has been used to simulate multidimensional detonation waves and to examine the suitability of parallel computer architectures for computing reactive flows. It has been found that the Connection Machine is a good platform for simulating unsteady, inviscid compressible flows, however efficient integration of the chemical rate equations on a parallel computer sometimes requires additional programming to properly manage the processor loads.

The flow behind a shockwave propagating into a hydrogen-oxygen gas has been simulated on a CM-2, CM-200, and a CM-5 using the same data parallel program.

In a reactive flow simulation, integrating the chemical species rate equations on a parallel computer architecture was found to be inefficient if the processor loads were not actively managed. Separate routines were written to balance the load among the multiple processors to achieve efficient utilization of the Connection Machine. The new load balancing algorithm is based on CM Fortran Library functions which create send addresses and perform gather/scatter operations on the unconverged grid points. Significant speedups are realized by balancing the chemistry integration such that the percentage of useful work conducted is maximized. The data parallel structure and implementation of CM Fortran functions provides a load balancing routine that is portable between the different architectures available in the CM-200 and CM-5.

1.2 NASA Ames Research Center:

The CM-5 system was installed at NASA Ames in the first half of January, 1993. The system was brought to user community during the second half of January. Average availability of the system has been approximately 95%, and usage is more than 50% of a 24 hour shift. The CM-5 configuration at NASA Ames consists of 128 nodes with vector units, 4 Control Processors and 1 I/O Control Processor, and an SDA with 48 drives. Three HIPPI channels and crossbar are expected to arrive in October. NASA Ames has also served as a beta site for new releases of many software systems, e.g., CMOST, CMFortran, C*, PNDBX, and CMAX.

The Ames user community began to explore MIMD features of new CM-5 system. Tim Barth and Sam Linton are in the process of implementing a turbomachinery unstructured code on CM5 (this code ran before on the Intel iPSC/860).

Work was also begun in a new direction of parallel scientific visualization. The CM AVS package was installed and tested rigorously at Ames. A new program which will visualize Saturn's ring is in the final stages of testing. The source of data is a parallel code which simulates Saturn's planetary, moons, and particles system (Creon Levit and Space Science Division). The visualization (by Arsi Vaziri and Mark Kremenetsky) is based on CM AVS software.

A number of major data parallel projects which used to run on the CM-2 system have been successfully reimplemented on the CM5.

CM3D: Dennis Jespersen, Creon Levit (NASA)

A compressible Navier-Stokes solver for use on multiple overlapping three-dimensional structured curvilinear grids. This code is a core for developing a production code for use by the United States aerospace industry.

AMESCEM: Michael J. Shuh (NASA)

This is a three-dimensional finite-volume time-domain electromagnetic code(FVTD) code. It is run on multiple block curvilinear grids so as to predict scattering from complex objects .

DNS (Direct-Navier-Stokes-Simulation): Nateri Madavan (NASA)

The objective is to perform direct numerical simulations of spatially-evolving compressible turbulence using high-order-accurate finite-difference techniques. The development of a DNS code is aimed at providing accurate turbulent inflow boundary conditions for use in spatial simulations of transition and turbulence. This code currently achieves about 750 MFLOPS performance in double precision on a 32K CM-2 and 128 node CM-5. This code requires so much memory that it can be implemented only on CM. The CRAY YMP works as preprocessor for the CM-5 in this case.

RANS (Reynolds-Averaged-Navier-Stokes): Nateri Madavan (NASA)

The focus of this project is on the highly compute-intensive end of the CFD application spectrum. RANS equations are solved in an implicit, time-accurate manner, using upwind schemes and zonal methodologies representative of current state-of-art in CFD. The major impetus for this research is a growing belief that MPP holds the key to developing future teraflop capability and the potential for meeting computer performance requirements of large scale scientific simulations.

PSICM: Leonardo Dagum (NASA)

The objectives of this project are to accurately describe high

altitude plume interaction phenomena and accurately simulate expanding flows starting either at the nozzle exit plane, or at a supplied starting surface. The core of this code is based on a direct simulation Monte Carlo method. Using a starting surface obtained from a Method of Characteristics solution for an Orbiter reaction control system (RCS) engine plume, the code demonstrated the existence of a plume/plume self-interaction shock for two engines separated by 69 feet. The self-interaction shock is a complicated three-dimensional structure and the calculation required the large memory and performance of the Connection Machine to be completed in a reasonable amount of time. The implication of a self-interaction shock for separation distances of 60 feet is highly relevant to the space station design.

Computational Fluid Dynamics on Connection Machine:

Horst D. Simon (NASA),

Mark D. Kremenetsky, John L. Richardson (TMC)

A two-dimensional implicit Navier-Stokes parallel procedure for an application to a compressible turbulent flow was developed along with the necessary parallel preconditioners and solvers. The preconditioning phase is crucial for the convergence of the developed procedures, and an approach to preconditioning for very large block banded unsymmetric linear systems based on computing of an approximate inverses to an original system was used. The algorithm exhibits a natural parallelism which can be effectively exploited on massively parallel machines. The developed methods were implemented on the Connection Machines (CM-2 and CM-5) using the CM Fortran language. Relevant publications include:

M.D.Kremenetsky, J.L.Richardson " A Parallel Unfactored Solver for Computational Fluid Dynamics," Proceedings of Parallel CFD '92 Conference, New Brunswick, NJ, May 1992
M.Grote, H.D.Simon., "Parallel Preconditioning and Approximate Inverses on the Connection Machine," Proceeding of the Scalable High Performance Computing Conference (SHPCC) 1992, IEEE Computer Society Press, Los Alamitos, CA 1992, pp.76-89

2. PLANNED ACTIVITIES FOR NEXT REPORTING PERIOD

Continuation of projects discussed in 1.1 and 1.2. See above for additional information.

3. MAJOR EXPERIMENTAL OR SPECIAL EQUIPMENT PURCHASED

- nothing -

4. CHANGES IN KEY PERSONNEL

- none -

5. INFORMATION DERIVED FROM MEETINGS AND CONFERENCES

-nothing to report-

6. SUMMARY OF PROBLEMS OR AREAS OF CONCERN

- nothing to report -

7. RELATED ACCOMPLISHMENTS SINCE LAST REPORT

- initial report -